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STRACT (Maximum 200 words)

The PDM or Particle Dynamics Method for simulation of clastic sediment motion has been used to study the motion of clastic sediment at the level of the individual particle. This technique can be used to assign properties to sediment beds like grain size and grain size distribution, grain shape, and so forth, and then to study the response of the system to specified external conditions such as levels of applied stress, slope angle of bed, or depth of water column.

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Final Report
to the US Army Research Office
on
Computer Simulation of Subaqueous Sediment Transport
Grant No. DAAL03-89-K-0163

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December 1992

Abstract

The PDM or Particle Dynamics Method for simulation of clastic sediment motion has been used to study the motion of clastic sediment at the level of the individual particle. This technique can be used to assign properties to sediment beds like grain size and grain size distribution, grain shape, and so forth, and then to study the response of the system to specified external conditions such as levels of applied stress, slope angle of bed, or depth of water column. A short discussion of preliminary results in the areas of sediment mixing, swash transport, and surface stability are given. Thus, vertical diffusion of sediment particles within the bed occurs due to shearing stresses even in the absence of erosion or deposition; it is thought that this effect may have importance to problems in contaminant transport in environmental engineering. The balance of sediment transport on a beach during swash and backwash is studied as a function of beach slope; the competition between friction and gravity produces equilibrium beach angles which are calculated explicitly within this model as individual sediment grains are dragged up and down the beach by the oscillatory water motion. In studies of stability of individual particles against applied surface stresses, we found that three dimensional results gave pivot angles about 10 degrees less than the corresponding study in two dimensions. Variation of grain friction coefficients produced little effect, except for very elongated grains which tended to slide rather than roll as their failure mode. Working of a bed by fluid shear prior to testing pivot angles showed that imbrication of modestly

elongated particles could lead to somewhat higher pivot angles.
Abstracts for preliminary reports on this work plus abstracts of
work already published are included in an Appendix.

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Introduction

The goals of the research supported under this grant were to develop new methods and models for understanding subaqueous sediment transport at a fundamental level. The main developments are sketched here. The title pages and abstracts of both published papers and unpublished reports are given in the Appendix.

The principal technique that we have pursued has been PDM, or the Particle Dynamics Method, in which the motion of hundreds to thousands of individual clastic sediment particles are followed by explicit integration of their equations of motion. The force between the particles are modeled by stiff "springs" (in compression) and a Coulomb-type friction law. Obviously, simulations at this level are not used to predict directly the larger scale sedimentary behavior of systems such as rivers or coastlines. Rather, they can be useful as tools for assessing the kinds of phenomena that clastic systems undergoing shear are likely to develop.

Most problems in subaqueous sediment transport can be divided naturally into two parts - the particle sector and the fluid sector. The particle sector, as mentioned, is studied by direct solution of the classical equations of motion, $F = ma$. Besides the contact forces and gravity, the force F exerted on each grain has contributions from the interaction with the fluid. For most of our work, this is modeled as a simple drag force that is a function of the instantaneous relative velocity between particle and fluid. The fluid motion itself

is computed using a simplified model in which thin layers of fluid glide over one another, exerting a frictional force on neighboring layers via eddy viscosity, and exerting drag on any sediment particle embedded in the layer. In this way, overall fluid plus particle momentum is conserved.

We feel that the PDM method is potentially an important tool for sediment studies because it is so general. The behavior of different sizes, shapes, densities, etc., can be studied, as well as the behavior of mixtures of particles with different properties. While the layered-fluid model is an especially simple one, the structure of PDM models will easily allow better fluid models to be used when they become available.

Published Results

In order that information on PDM modeling in a sedimentology context be made widely available, we have written up the method in substantial detail in a paper to be published in Water Resources Research ("Multi-Particle Simulation Methods Applied to the Micromechanics of Bedload Transport"). Further discussions and developments have been or will shortly be published in other journals, conference proceedings and book chapters ("Basic Physical Models in Sediment Transport"; "Transport of Granules by Wind and Water: Micromechanics to Macromechanics in Geology and Engineering"; "Grain Scale Simulations of Loose Sedimentary Beds: the Example of Aeolian Saltation", and "Discrete Mechanics").

Unpublished Results

In addition, three separate applications of this method have been carried out but are not yet published. Abstracts are given in the Appendix.

In the first of these applications, the depth of the bedload layer is studied as a function of shear stress ("Mixing of Sediments During Bedload Transport"). As flow velocity and hence shear stress increase, bedload mass flux also increases. At first this increase is due mainly to the increased speed of transported surface grains. As shear stress increases, however, the layer of sediment undergoing bedload transport increases in thickness. In order to shear previously stationary grains, the bed must dilate, and the dilatation allows vertical particle diffusion throughout the sheared layer. Consequently, grains which rested initially on the surface will soon be spread evenly through a vertical distance equal to the sheared depth. Correspondingly, initially buried particles can diffuse to the surface even if there is no net erosion. These results are thought to be relevant to environmental concerns over sequestering and exhumation of contaminated sediment on a river or stream bed.

In another application, a simplified model of wave swash on a beach was used to investigate the role of slope and infiltration rate on sediment transport ("Microgranular Model of Bedload Transport During a Swash-Backwash Cycle"). A nearly uniform swash event was modeled as a stack of thin fluid layers which were initially impelled up the beach, eventually coming to rest under the combined

effects of gravity and friction, then finally reversing direction and moving back down slope. Since the layered-fluid model is inherently time dependent, the vertical velocity structure of the swash is complex; part of the fluid near the surface of the flow is still moving upslope when the fluid near the bed has already begun to move back out again.

During the upslope motion, surficial sediment grains are dragged upslope by the swash, and, when the flow reverses, they are dragged back downslope. Whether there is a net upslope or downslope component of sediment motion (that is, net deposition or erosion) depends upon the bed slope. At small angles, there is a small net upslope motion, since the backwash is slightly weaker than the swash, due to the effect of friction. At larger beach slopes, this effect is insufficient to overcome gravity, and there is net outwash of grains. We also studied the effects of infiltration of the fluid. Infiltration has a profound effect on net sediment transport, tending to increase upslope sediment transport and hence beach slope, an effect in agreement with the observation that coarse sediment beaches tend to be steeper than fine sediment beaches.

Finally, we have looked at the "pivot angles" or "friction angles" of individual stationary grains in both two and three dimensions ("The Pivot Angle of a Loose Particle on a Bed of Fixed Particles"). The pivot angle is a measure of the stability of a granular bed. In 3D, we show how the geometry of the surface of random grain packings controls this important angle. We explicitly compare two and three

dimensional calculations of this angle in order to give some idea of the types of errors likely to be encountered in 2D models of bed stability. As expected, in three dimensions pivot angles are substantially smaller than in 2D, because particles can escape from their resting positions via the valleys between bed particles, while in 2D, these particles must go "over the top" of neighboring grains to escape. We have also looked, in 2D, at the effect of variations in the grain-grain friction coefficient on the stability of non-spherical particles. Friction seems to be relatively unimportant, except at larger values of grain ellipticity, where sliding instead of rolling begins to be an important mode of grain displacement.

One may conclude from the range of applications that PDM methods represent a general approach to the study of specific issues of sediment transport at the microscale level. While these methods are not intended for direct large scale applications, they provide insight into diverse aspects of grain mechanics and help to augment our knowledge and understanding of clastic sediment transport.

Appendix

Title Pages and Abstracts of Published Papers and Preliminary Reports (to be Published)

Mixing of Sediments During Bedload Transport (Preliminary Report)

Microgranular Model of Bedload Transport During a Swash-Backwash Cycle (Preliminary Report)

The Pivot Angle of a Loose Particle on a Bed of Fixed Particles (Preliminary Report)

Multiparticle Simulation Methods Applied to the Micromechanics of Bedload Transport (Z. Jiang and P. K. Haff, *Water Resources Research*, in press)

Basic Physical Models in Sediment Transport (P. K. Haff, Proc. *Coastal Sediments '91*, ASCE, vol. 1, ed. N. Kraus, et al., pp1-14, 1991)

Transport of Granules by Wind and Water: Micromechanics to Macromechanics in Geology and Engineering (P. K. Haff, Z. Jiang, and S. B. Forrest, *Advances in Micromechanics of Granular Materials*, Elsevier, NY, H. H. Shen, et al., eds, pp373-379, 1992)

Grain-Scale Simulations of Loose Sedimentary Beds: The Example of Aeolian Saltation (*Sedimentology*, in press)

Discrete Mechanics (chapter in *Granular Matter: An Interdisciplinary Approach*, ed. A. Mehta, Springer-Verlag, in press)

Mixing of Sediments During Bedload Transport

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December 1992

Abstract

In this paper, vertical subaqueous sediment mixing and its relationship with shear stress are studied. We studied two different cases: fine gravel ($D_{50} = 5\text{mm}$) and medium sand ($D_{50} = 0.8\text{ mm}$) under different shear stresses. When shear is applied to the sediment bed, the layer of sediment undergoing shear dilates, and during this dilational event, individual sediment particles can diffuse throughout the dilated volume. Applications to environmental engineering and biological problems are envisioned. For instance, if the topmost grains on a sediment bed are contaminated, then a shear event sufficient to cause shearing to a depth h will also cause diffusion of contaminated material to that depth. Likewise, buried material, if disturbed by shearing, can diffuse to the surface of the sediment bed. This diffusional motion occurs within a few seconds in most cases. This effect is distinct from burial or exposure of material by deposition or erosion of sediment, as vertical mixing through diffusion occurs even in the absence of erosion or deposition. The mixing depth is predicted to be proportional to the applied shear stress, and to be independent of the sediment grain size.

Microgranular Simulation of Bedload Transport During a Swash-Backwash Cycle

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Abstract

The Particle Dynamics Method, or PDM, is used to study the behavior of sediment during swash-backwash events on a beach. Water rushes up the beach and back in response to breaking waves and gravity. Friction with the bed slows this swash/backwash cycle on both its upslope and downslope trajectories. Friction tends to weaken the backwash leg relative to the upslope swash leg of the trajectory, while gravity tends to strengthen the downslope backwash leg. At low slope angles friction prevails, and net sediment transport is upslope. At larger angles, gravity prevails, and net sediment transport is seaward. We estimate the angle of beach stability by considering the motion of a uniform packet of fluid as it moves up and down the beach. The motion of individual sediment particles are followed during this process using PDM. The swash itself is modeled as a set of uniform slabs of fluid which can slide with respect to one another. Total momentum of fluid plus sediment is automatically conserved.

**The Pivot Angle
of a Loose Particle
on a Fixed Bed of Particles**

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December 1992

Abstract

The pivot angle is the minimum angle with respect to the horizontal that a fixed bed of particles must be tilted in order to move a loose individual particle resting on that bed. The motion of the particles in this study of pivot angles is simulated by a Particle Dynamics Model which calculates the motion and collision of individual sediment particles. A method for calculating the pivot angle is derived for a three dimensional bed of frictionless spheres with diameters of little variance. This method reproduces the experimental results of Li and Komar and the theoretical results of Eagleson and Dean for a close packed bed. This method can also be used to compute pivot angles for non-crystalline arrangement of particles. The pivot angles of three dimensional spheres are up to 10° smaller than the pivot angles for 2D circular particles. In addition to spherical particles, elongated particles were also considered. The motion of elongated particles has an increasing sensitivity to the coefficient of friction (f) with an increasing diameter of the surface particle relative to the diameter of the bed particles, as sliding becomes more important than rolling. The imbrication of particles is simulated via a moving fluid that imposes a shear stress on a bed of elongated particles. The resulting bed produces somewhat higher pivot angles than the non-imbricated bed. Using studies like these we can make quantitative estimates of

the consequences of constructing models with idealized frictionless, two dimensional, circular particles.

**Multi-Particle Simulation Methods Applied to
the Micromechanics of Bedload Transport**

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August 1992

Abstract

We solve the Newtonian equations of motion to follow the trajectories of each of a large number of two-dimensional circular bedload particles as they move in response to stresses exerted by an overlying fluid. The fluid is modeled as a moving layer or "slab" which exerts a velocity dependent drag force on embedded particles and satisfies its own momentum balance equation. Bedload mass flux and hop length and hop height statistics of simulated beds resemble those observed in the laboratory. By marking particles originally residing on the surface, vertical mixing of sediment is investigated. An injection of fine particles into a bedload system of coarse particles under traction illustrates the early stages of the evolution of sedimentary stratigraphy. Friction angles and their distribution are investigated as a function of bed transport history and particle size. The main thrust of the paper, however, is to describe and test a microscopic bedload model which engineers, geologists and biologists may find useful for applications where particle arrangement and relative particle motion are important.

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BASIC PHYSICAL MODELS IN SEDIMENT TRANSPORT

Peter K. Haff¹

Abstract: Basic particle dynamics and cellular automata micromodels of clastic sediments are described and applications are illustrated in the areas of aeolian saltation, bedload transport, size segregation in shear flows, dry granular flows and aeolian bedform generation.

INTRODUCTION

Many clastic sedimentation systems can be divided into two constituent subsystems - called here the particle sector and the fluid sector. The particle sector consists of the solid grains while the fluid sector includes the air or water in and around these grains. The motion of the solid grains is governed by the classical equations of motion, e.g., Newton's equations for the motion of the center of mass of each grain and Euler's equations for rotational motion about the center of mass. The forces and torques which enter into these equations arise from gravity, from the mutual interaction between grains at their contacts, and from fluid pressure and drag effects. If we know these forces, then the classical equations can in principle be solved to obtain the positions, orientations and velocities of the grains as functions of time. Workstation computing power is sufficient to follow the motion of hundreds to thousands of grains for times of several seconds in the particle world. Computer simulations of this sort, dubbed the Particle Dynamics Method (PDM), can therefore be useful for investigations where the behavior of a relatively small number of particles over short periods of time is of interest. This might include questions of bed surface roughness, packing, sorting, porosity, transport mode (saltation, rolling, etc.), forces between grains, deformation and failure mechanisms, and so forth.

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Transport of Granules by Wind and Water: Micromechanics to Macromechanics in Geology and Engineering

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Abstract

We present two examples of micromechanical simulations and show how the calculations can be used to draw useful conclusions at the macroscopic level. In bedload transport by water we examine the mixing-depth of sediments undergoing shear-traction. In transport of dry sand grains by wind we examine the development of periodic bedforms and the burial and preservation of bedding surfaces.

1. Introduction

Micromechanical investigations of granular systems, in which the behavior of a small number of "representative" grains is studied in great detail, are sometimes used as the basis of an extrapolation to a macromechanical regime, where the motion of a large number of grains is involved. This transition is often accomplished through the calculation of constitutive relations, in which average grain behavior at the microlevel is encapsulated in a concise mathematical statement relating macroscopic variables. The calculations of the constitutive law can be either analytical [1] or numerical [2], but in either case the underlying assumption is that there exists a partial differential equation describing the macrophenomenon and that the computed or otherwise inferred constitutive relation can be embedded in this PDE. This linkage of the microworld to the macroworld has proven to be a central concept in the classical description of the properties of certain materials, e.g., Newtonian fluids, and it has also provided much insight into some aspects of granular flow - especially high-speed flows when the assumptions of kinetic theory can be applied [1,3-5].

There are, however, examples of granular materials where either the PDE is unknown or where it does not exist, yet where through experiment or computer simulation we have some knowledge of granular behavior at the microlevel. The question then becomes how to use this knowledge at the macrolevel. For instance, high-density granular assemblies often

**Grain-Scale Simulations of Loose Sedimentary Beds:
The Example of Grain-Bed Impacts in Aeolian Saltation**

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ABSTRACT

Sediment transport by wind is one of many processes of interest to the geomorphologist in which grain-grain contacts play an important role. In order to illustrate the modeling of collections of frictional, inelastic sedimentary grains with the particle dynamics method (PDM), we use the grain impact process in aeolian saltation as a specific example. In PDM, all the forces on each particle are evaluated at a sequence of small time steps, and the Newtonian equations of motion are integrated forward in time. Interparticle forces at grain contacts are treated as springs with prescribed stiffness (normal force) and by a Coulomb friction law (tangential force); particle inelasticity is represented by spring damping. The granular splash resulting from saltation impacts is assessed for sensitivity to the choice of grain properties, and the integration time step. We find that for the range of impact speeds and impactor masses relevant to aeolian settings, grain splashes are relatively insensitive to grain stiffness, grain inelasticity, and grain friction, and that the pattern of ejection from the bed is largely controlled by bed microtopography. A large set of impact realizations involving a variety of impact points on a small set of target beds is used to collect the appropriate statistics to describe the stochastic splash process. The splash function representing these statistics is then available for use in longer time-scale calculations, such as the evolution of the saltation curtain. The details given here will enable the interested reader to adapt PDM modeling to other types of clastic sedimentary systems.

Discrete Mechanics

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Abstract

Several computer simulation methods for modeling mechanical systems composed of disjoint pieces are discussed, including hard-sphere models, cellular automaton models, and particle dynamics models. Hard-sphere models are useful where a kinetic picture of a rapidly deforming granular medium is valid, but fail for systems where enduring particle contacts are important. Cellular automaton models can be used to advantage where it is important to simulate the motion of large numbers of particles (systems containing as many as 10^6 elements have been studied). Particle dynamics models (PDMs) include those in which detailed force models are invoked at particle contacts. In PDMs the motion of individual particles is evolved by solving the corresponding Newtonian equations of motion. These models can handle enduring contacts as well as arbitrarily large strains, and are the most general of the discrete mechanics models.